
Defense Threat Reduction Agency CB Modeling and Simulation Futures Workshop



ADVANCED SYSTEMS AND CONCEPTS OFFICE

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Executive Summary

Modeling and simulation of chemical and biological agent threats is a mission-critical capability of the Defense Threat Reduction Agency (DTRA). The DTRA convened a two-day workshop of technical experts and government leaders to study the current technical status and possible futures of the CB modeling and simulation field. The guiding workshop theme was the “practical” creation of actionable knowledge through modeling and simulation. The goal of the workshop was to identify and assess opportunities for progress across the broad spectrum of relevant technical areas. This exercise was intended to provide a framework for subsequent program development activities for CB modeling and simulation by DTRA through the Joint NBC Defense Program and interagency partnerships.

A taxonomy for describing CB modeling and simulation was developed, and five distinct application domains were identified, as follows:

- Acquisition
- Mission Analysis
- Consequence Management
- Forensic Reconstruction
- Exercise and Training

Within these domains, the following technical and operational discipline specialties were assessed, shown here with some relevant questions:

- **Intelligence integration and source term:** What is the quantitative nature of the event(s) initiating the CB hazard condition? How much can be known prior to a release, during an event, or in forensic reconstruction of a release event?
- **Transport, dispersion, fate, and terrain:** What happens to the agent after release, through dilution, transformation, deposition, re-suspension, and terrain-related processes?
- **Weather (atmospheric dynamics):** How could this discipline more fully enable CB hazard prediction? Weather prediction and data acquisition can provide data on meteorological phenomena playing central roles in hazard evolution.
- **Dose-response:** How are humans, animals, and plants affected by given exposures to agents?
- **Population epidemiology:** How do effects of CB agent releases propagate and persist in exposed populations?
- **Agriculture and biota:** What are the strategic defense issues, and the role of the DoD M&S program, in view of the potential for both accidental and deliberate introduction of CB agents?
- **Materiel:** The impact of CB agents on defense materiel, transport, and support systems could be significant. Do we understand the key uncertainties in this area?

The workshop produced a general consensus evaluation of technical and operational modeling disciplines. Understanding the knowledge creation challenges that are posed by each domain, the

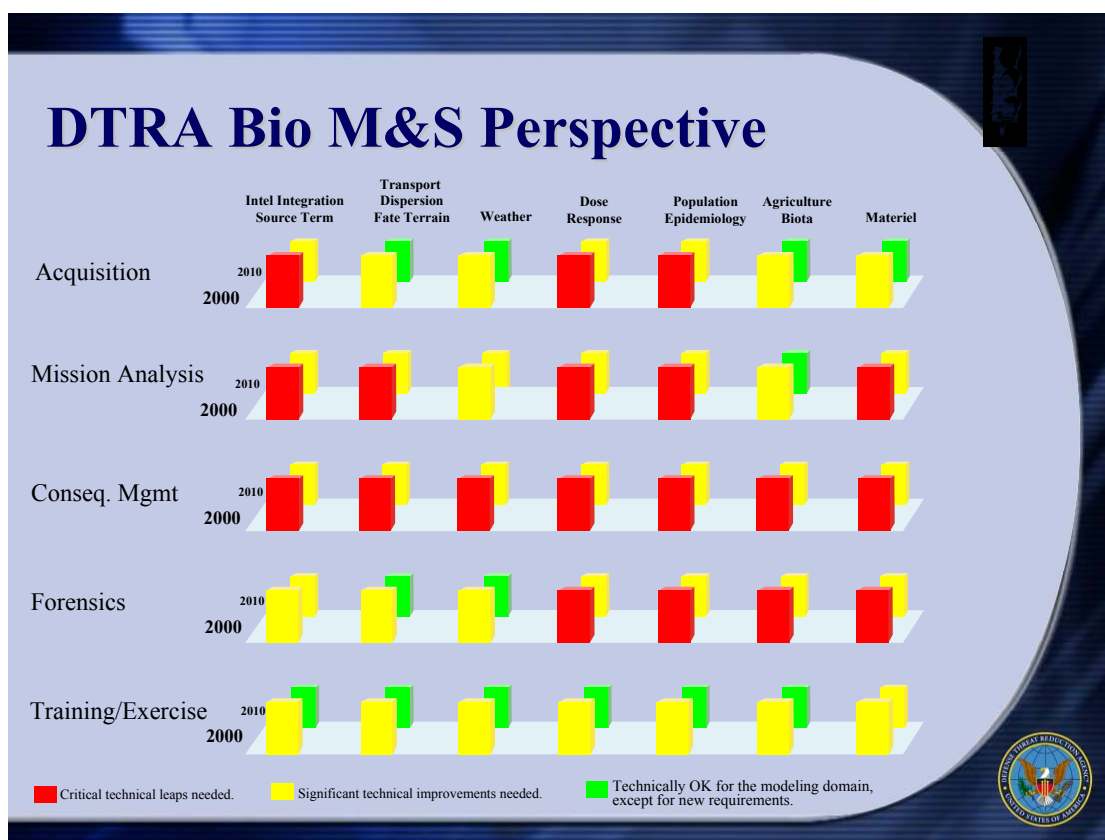
participants assessed the constituent disciplines for their current states and the opportunities for progress. On the final day of the workshop, panel members ranked the levels of scientific challenge posed by the modeling specialty disciplines.

Table E-1: Grading the Level of Scientific Challenge per Specialty Discipline

Color	Meaning
Red	Critical technical leaps needed
Yellow	Significant technical improvements needed
Green	Technically proficient for the modeling domain. New requirements may change this to “red” or “yellow.”

Expected improvements by 2010 were identified, as shown in the following figure. This future status presupposes whatever appropriate funding for the necessary improvements to occur. The colors are merely an indication of the scope of the purely technical challenges, and do not reflect fiscal or other constraints on progress.

Figure E-1: Current State and Expected Improvements by 2010



Based on this consensus ranking, we suggest that certain technical specialty areas are worthy of development through focused programs. Priority efforts in these areas offer the greatest potential benefits in actionable knowledge for critical decision support. Advancing the state of the art of CB M&S in the directions noted here will directly support and enable the DTRA mission.

Table E-2: Grading the Level of Scientific Challenge per Specialty Discipline

<i>Technical Specialty</i>	<i>Priority for Development</i>
Population Epidemiology	CRITICAL
Dose Response	CRITICAL
Materiel	HIGH
Source Term	HIGH
Transport, Dispersion, Fate, Terrain	MODERATE
Agriculture and Biota	MODERATE
Weather (atmospheric dynamics)	MODERATE

The workshop participants consider all the specialty areas worthy of enhanced effort. However, from DTRA's unique perspective, our relative assessments primarily reflect the expected achievements of other Federal agencies in development of complementary technology. For example, weather is rated as only a MODERATE priority, as this discipline is very highly advanced in relative terms in its contributions to CB M&S. Critical investments are still needed to integrate technological advances and discoveries in weather science to assure validity of the entire "end-to-end" process.

Developing the capability for modeling in the agricultural and biota domain would likewise be considered a very high priority area for the appropriate agencies. Continued collaboration and cooperation between the DoD, academic, and interagency programs shows incredible promise for synergy and economy.

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In addition, DTRA appreciates the workshop participants for providing summary presentations to baseline our current CB Modeling and Simulation Capabilities, providing the framework for subsequent discussions, especially Dr. Allan Reiter, DTRA, and David Grenier, Naval Surface Warfare Center, Commodity Area Manager for M&S for the Joint NBC Defense Program.

Ms. Madhu Beriwal of Innovative Emergency Management, Inc., served as facilitator and catalyst for the two-day workshop. Her vision for the workshop and invaluable contributions are sincerely appreciated. The workshop was developed and managed for DTRA by Dr. Peter Merkle. Logistics support was provided by Triumph Technologies. Thanks to Tim Bauer, LTC Ed Kertis, and MAJ James Wentworth for key contributions to workshop development.

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Introduction

Dr. Jay Davis (Director, DTRA) opened the Chemical Biological (CB) Modeling & Simulation Futures Panel by posing the following question: “It is expected that for the first 12 to 60 hours after a chemical or biological event, the response would be based on modeling. How confident are we that we can provide actionable information from our models?” Very difficult problems exist, such as confident low-level exposure risk determinations for combat commanders. The operational analysis challenge is the production of actionable knowledge, resulting in real-time theater and command awareness of the past, current, and future states of the WMD theater, down to the unit level. There should be consideration of consequence management, and how we interface the deliberations and conclusions of the workshop into decision modeling.

Dr. Davis asked the workshop to consider the problem from end to end, breaking it down into "boxes" such as source term, atmospheric transport, on through to dose response, morbidity and mortality. Can we describe what we know about each box, and what R&D would improve it? What are the targets of opportunity? If there were a billion dollars available for investment, where could the greatest benefit be gained in creation of actionable knowledge for operators? For example, should we invest more in modeling transmission of infectious disease, or in modeling the atmospheric transport of microbes of a particular size range? Can we bound the limits of knowledge, describing inherent uncertainties such that "the best we will ever get" can be identified? There are limits to knowledge, given testing constraints. Dr. Davis described the challenge as one of two or three most difficult scientific problems he could imagine.

Points raised during subsequent discussion included:

- Dr. Davis' interactions with top-level Federal officials often include describing the uncertainties of the modeling process that these individuals may "consult" to make real-world decisions. A correct "scoping" of the problem of uncertainty by the workshop will have great impact.
- When communicating the results of models, political boundaries as well as geographic boundaries matter to the first responder, and to a civil or military leader.
- A community roadmap is a step forward, and should highlight the degree of multidisciplinary difficulty in advancing the state of the art. Optimizing one "box" does not mean that knowledge has been created in the end to end modeling equation (from source to ultimate effects).

In response to Dr. Davis' tasking, the CB Modeling & Simulation Workshop focused on current capabilities as a foundation for modeling and simulation, and it sought to identify specific opportunities for improvement.

Mr. David Grenier, Joint Service Materiel Group Commodity Area Manager for M&S, provided a background summary of the organizational relationships and initiatives for CB Modeling within the DoD's Joint NBC Defense Program, described in the Master Plan (in draft). There will be a system of M&S systems, completely interoperable, with one user entry point. The overall system will be responsive to user needs and accountable to DoD accreditation authority. The requirements and operational capabilities areas were summarized. Specific requirements are the foundations of four major

programs for new systems: Joint Effects Model (JEM), Joint Simulation Federation, Joint Prototyping System, and Training Systems.

Dr. Allan Reiter of DTRA portrayed the CB Modeling and Simulation field as a linked array of many specialty disciplines:

- Source Term
- Intelligence
- Weather
- Transport, Diffusion and Fate
- Terrain
- Dose Response
- Population and Epidemiology
- Agriculture and Biota
- Materiel

Dr. Reiter's presentation was used as a framework for subsequent workshop sessions. Each of these discipline areas was discussed at the workshop. Participants noted current capabilities and available scientific opportunities. While it is not possible within the scope of this paper to document discussions in detail, we attempt here to summarize the central or important themes.

By design, the CB Modeling and Simulation Futures Workshop did not focus on the capabilities of any specific models. The workshop intent was to review the current modeling capabilities as a whole and identify the high-payoff areas where investment may be warranted.

To obtain actionable results requires an understanding of the overall needs of actors under varying conditions. The workshop developed a taxonomy of modeling domains to discuss modeling needs. These domains are shown in the figure below.

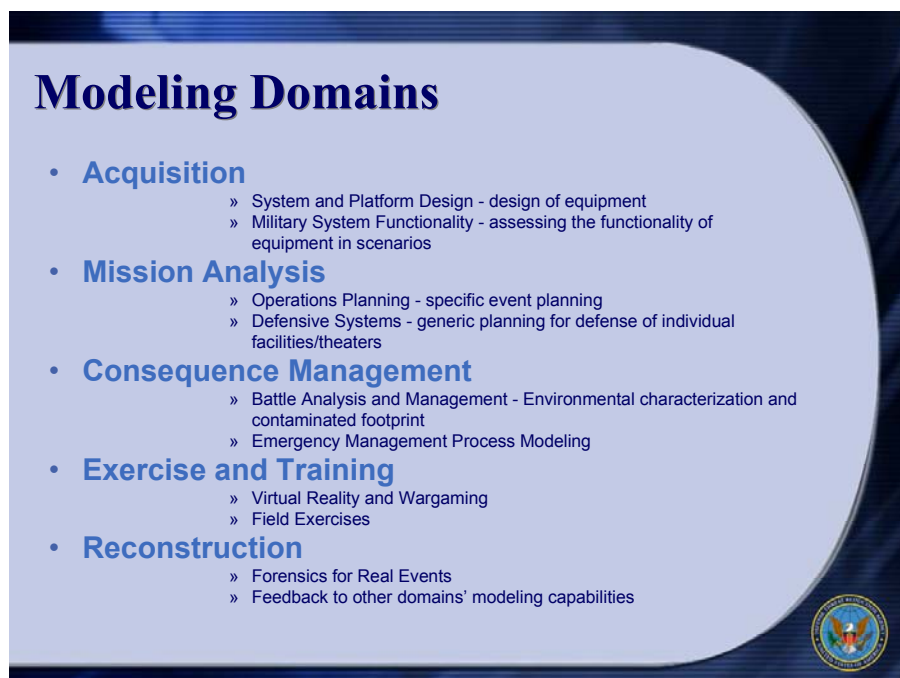


Figure 1: Modeling Domains and Relevance to Other Domains

Intelligence and Source Term

Background

The workshop participants recognized that for “end-to-end” modeling, the starting point is generally the *source term*, or *the quantity and mode of chemical or biological agent release*. Knowledge of the specific agent, as well as the amount of release and the mode of release is necessary to subsequent modeling. The source term is potentially knowable to some useful approximation.

The consensus of the workshop participants was that, lacking real-time observation and sampling, intelligence will never provide complete certainties in determining a source term. Although efforts to reduce the source term uncertainties can be very productive, the problem can only move from a status of “red” (can’t make a difference) to “orange” (could make marginal improvements). The advent of agent and weather sensor networks linked with battlefield hazard and warning systems is eagerly anticipated.

Recommended Scientific and Technical Directions

There was consensus that full source term knowledge will be lacking to some degree, and that determination of the source term is a vital

step in an “end-to-end” modeling effort. Participants emphasized the use of the science and technology (S&T) tools listed below to manage the uncertainty. Each of these tools is discussed in the following sections.

- Probabilistic or Uncertainty-Based Modeling
- Quantitative Risk Assessment (QRA) and Probabilistic Risk Analysis (PRA) for Source-Term Determinations
- Parameter Sensitivity Modeling
- Test Data for Model Validation

Probabilistic or Uncertainty-Based Modeling¹

Uncertainty is inherent at many stages of “end-to-end” modeling. Various phenomena characterized in models may have ranges of behavior, i.e., they are stochastic. Uncertainty also arises from a lack of knowledge about certain phenomena; this is subjective uncertainty.

Probability is the most generally-accepted mathematical formalism for representing uncertainty. For source term modeling, there is uncertainty about *what the source term might be* and *the degree of confidence in the modeled source term*. As more information is available, the probabilities assigned to the source term can be varied. This is the Bayesian view of probabilities.

Various analytical methods are used to parsimoniously propagate the uncertainties in a model to the model-predicted outcomes. One of the methods, Monte Carlo simulation, was discussed at the workshop. Monte Carlo simulation is a technique for selecting a moderately large random set of samples to characterize the known uncertainty surface. The sample size of a Monte Carlo simulation may determine, to a large degree, the resulting accuracy. With a Monte Carlo simulation, it is not necessary to identify the instantiation or discrete values for each variable. Only the continuous distribution or the range of possible source terms needs to be identified. In addition, the sample size can be varied for lower accuracy and faster output requirements. This technique is less demanding both on computational requirements and knowledge requirements.

Dr. Steve Hanna advised that there have been several dose reconstruction efforts at Department of Energy (DOE) National Labs and the Centers for Disease Control (CDC). These efforts have

¹ We are indebted to Dr. Steve Hanna for his assistance with the documentation in this section. See also IDA Paper P-3554 on *User-Oriented Measures of Effectiveness for the Evaluation of Transport and Dispersion Models*

almost always used a Monte Carlo uncertainty approach, applied to the end-to-end modeling system. The Environmental Protection Agency (EPA) has a growing interest in Monte Carlo uncertainty methods and has prepared a Guidelines Report.² George Mason University has recently conducted Monte Carlo uncertainty analyses for a regional ozone modeling study³ and is also initiating a Monte Carlo uncertainty study for mesoscale meteorological models.

There was some concern expressed that battlefield commanders did not know how to interpret probabilistic information. Outputs from probabilistically-derived hazard predictions should be carefully designed to portray results effectively to non-specialists.

QRA and PRA for Source Term Determinations

In the watershed “Rasmussen Report” of 1975, the nuclear industry has developed and refined a structured set of protocols for conducting PRAs (also known as QRAs, or Quantitative Risk Assessments, in other industries).⁴ The PRAs use a combination of event-tree and fault-tree analysis to identify the sequence of events associated with a universe of “accidents,” to calculate the expected frequency of releases, and to determine the release characteristics (e.g., size and timing) of each potential release. Since the “Rasmussen Report,” the PRA/QRA approach has become *de rigueur* in a variety of industries.

The PRA/QRA techniques can be applied to CB source term modeling to identify a large series of potential releases. This modeling, the panel expressed, could be especially relevant for scenarios involving industrial facilities and materials.

The PRA and QRA methods use stochastic uncertainty, i.e., the system may behave in different ways. For CB source term, given the nature of a weapon system, it can be stated that there is still uncertainty about how the weapon system may function in actual deployment. Therefore, the two techniques of Monte Carlo simulation and PRA/QRA cover two separate underlying sources of uncertainty: *uncertainty of knowledge* and *uncertainty of actual system behavior*.

Parameter Sensitivity Developed for Modeling “Short Cuts”

Models are approximations of reality. A model defines the real domain through the deliberate selection of the variables or parameters characterizing the domain to be modeled and the range and resolution of each variable in the system. Many CB Defense models define a

² Chang, 1997. This report is obtainable from the EPA web site (www.epa.gov).

³ Hanna et al, 2000.

⁴ Rasmussen, 1975. Nuclear Regulatory Commission, 1990 (NUREG 1150)

spatial grid for calculations; this grid can be as coarse or fine as necessary to enable modeling for system behavior. Model calculations can be performed at very small, incremental time steps or at large time steps. A further refinement is the use of adaptive grids in both time and space domains.

Model outcomes *can* be highly sensitive to grid parameters. One erroneous expectation is that a finer grid produces the highest fidelity model prediction. This raises the computational burden and reduces the flexibility needed to adopt models for use in the various applications across the modeling domains.

Greater accuracy and precision for input parameters does not always yield higher model fidelity. Very simple systems of equations may produce complicated system dynamics: for certain systems, even differential changes in the values of input parameters or boundary conditions will produce first-order changes in model predictions.

Workshop participants stressed the need to conduct parameter sensitivity modeling to allow the best cost-benefit tradeoff between computational complexity and confidence in model outcomes. Any CB model can be subjected to a sensitivity analysis in which variables are varied systematically to examine the effects on predictions.

Test Data for Model Validation

Test data are needed to ensure that source models provide reasonably accurate estimates of source terms. In many cases, highly instrumented tests are conducted which allow very complex, small-scale models to be developed (for example, the detonation of a chemical munition bunker). The need for data is as problematic as the need to develop the actual source models. Any consideration of testing of actual chemical or biological weapons for defensive purposes, such as developing effects models, is proscribed or otherwise regulated by treaty or statutory provision. Adaptation of safe and valid simulant testing procedures is possible, and leverage may be gained from non-defense discipline studies (such as EPA air quality programs). Passive data collections such as monitoring volcanic plume or forest fire smoke dispersion patterns from "known" sources are useful. Development of first-principles models sans testing data is a worthy goal (compare with the nuclear stockpile stewardship modeling efforts). One approach to the source term problem is a hierarchy of models suitable for specific applications, such as acquisition, training, effects, forensics, and varying in fidelity requirements. The ability to integrate real-time information (sensors, human information) is desirable.

Atmospheric Dynamics (weather at many scales)

Current Capabilities and Initiatives

"Scientists engaged in mesoscale and microscale meteorology research are poised to make major progress on improving forecasts of precipitation, and accounting more accurately for mesoscale and microscale processes in models of the climate and weather. This progress is made possible by recent advances in observing systems, computers, and theoretical understanding."⁵ Workshop participants concurred with this statement by the National Center for Atmospheric Research. Compared with some areas considered in this Workshop, weather modeling is a mature discipline. Weather models are available for varying scales, from detailed microscale models to mesoscale models, to global climate models. For most modeling applications in the Department of Defense (DoD) arena, mesoscale models are of greatest import. The integration of sensor networks into mesoscale modeling capabilities is an important challenge.

The U.S. Navy capabilities for military support (NOGAPS, COAMPS, TAMS/RT models) are constantly engaged in weather prediction, validation against observations, and distribution of products to users. Current requirements for these services exceeds resources. The Naval Research Laboratory has a "telescoping strategy" to provide global scale down to tactical "nowcast" capability. Adaptation of mesoscale models from one site to another is not simple, as unique local phenomena are the rule. Mesoscale models are now being integrated onto military platforms such as ships. This is expected to provide a forward-deployed capability to model the effect of releases and their spread. (Note that "real time" should be considered 1/20th of simulation time, that is, a 24 hour forecast should not take more than about 1 hour of computation time.)

Computing power has increased exponentially in the last several decades. However, the computing burden remains a real constraint for the modeling of atmospheric processes. Grid or cell size, one of the variables having a powerful effect on model outcome accuracy, is important for modeling contaminant transport; it is also important for proper characterization of atmospheric processes. If the grid size is too large,⁶ smaller-scale atmospheric phenomena are not modeled

⁵ NCAR, October 2000

⁶ The same problem occurs if the time scale is too coarse.

well. However, a smaller grid size raises both the data requirement and computing burdens.

Some research has been conducted on optimal grid resolution. This research indicates that a grid size of 4–5 kilometers for mesoscale models may be sufficiently detailed for a number of successful modeling applications. Smaller grid sizes may be recommended only for special cases, such as modeling for urban environments or terrain with severe natural gradients. Smaller grid sizes nevertheless require more detailed physics treatments of atmospheric processes to provide more accurate forecasts. Adaptive grids pose challenges for scale-merging in the fundamental physics as well as software development.

Weather models are sensitive to "start" states specified at model initiation. The state of the atmosphere at the start of the forecast period is not precisely known, and any model initiation includes some uncertainties. Ensemble forecasting is increasingly being used to encompass this uncertainty. In ensemble forecasting, successive model runs are initiated by perturbing initial conditions, each perturbation capturing some of the total range of known uncertainty. Ensemble modeling of initial atmospheric variables was also applied to forensics modeling of the Khamisiyah event.

Atmospheric forecast models provide many outputs; however, transport and diffusion models currently use a very limited set of these data.⁷ Windfields and temperature are commonly used to drive the pollutant transport and diffusion.

Urban areas pose a significant modeling challenge. Comprehensive validation of urban windfield models is in its infancy.⁸ Complex terrain also occurs in hilly areas, coastal areas, and on islands. Urban areas and other complex terrain areas need a new generation of models. Getting to "green" (having a robust modeling and simulation capability) in urban modeling, according to workshop participants, will be difficult.

The land-sea interface is an area of great climatic complexity. About 80% of the world's population lives at or near a coastline. This combination of factors calls attention to both the importance and the difficulty of producing "actionable knowledge" for coastal regions.

⁷ Hanna, Yang and Yin, 1999

⁸ Tehranian, Lohner and Hanna, 2000; Camelli and Lohner, 2000; Hanna and Britter, 2000; Hanna, 1999

Another area of challenge is to model the dispersion of contaminants within buildings. Many models exist today with varying capabilities to model indoor air flow. Since most people spend 90% of their time indoors in buildings, exposures to CB agents might predictably be expected to occur indoors. Air exchange with outside air for various classes of buildings and specific, well-defined buildings types to be understood by CB M&S developers. These modeling efforts must support multiple decisions/actions, such as which areas are contaminated, how quickly they are contaminated, when should shelters be abandoned, and dosages to human occupants. Exploration of existing codes developed for fire safety and HVAC engineering is warranted.

Scientific and Technical Directions

Integrated Atmospheric Processes, Transport, and Diffusion Modeling

The workshop participants recommended that the semantic distinction between the terms “weather” and “transport and dispersion” be slowly eliminated. This distinction is a carry-over from the days when weather models provided wind field data to drive separate dispersion routines. In practice, this distinction caused difficulties because many of the basic data needed by the dispersion routines were not archived by the weather forecasting community. In fact, current DoD models appear to use very little data from the “weather” models.

This problem was solved within the civilian National Oceanic & Atmospheric Administration (NOAA) many years ago. The next generation of civilian mesoscale models will solve all such problems by combining the transport and dispersion capabilities with the forecast codes. A number of civilian models already integrate the weather and transport and dispersion modeling in a single package.

Testing of “End-to-End” Models

These “end-to-end” models should be tested to ensure that with all atmospheric systems characterized, the end-to-end, integrated meteorological and plume model provides valid predictions.

Ensemble and Probabilistic Modeling

As ensemble and probabilistic modeling approaches are used, these powerful techniques can be applied to the end-to-end sequence of events, from the source term event through dispersion processes and the ultimate fate of the CB agent hazard.

Modeling Approaches

The future of Gaussian plume models is limited. Even with rapid advances in the near future, “real time” application of CFD codes is not feasible (excluding advanced planning for special events). The

CFD discipline does permit unique insights into dynamic effects on length and time scales of interest to command elements. At larger scales, the representation of turbulence in numerical weather prediction models, very critical surface fluxes, transport of solids in airflows, and utilization of sensor data are research needs. More validation work at a resolution of ~ 1 km is needed.

Adaptive Gridding

Despite the availability of higher computing power, trade-offs must be made between speed and accuracy. Areas of system complexity within the geographic domain to be modeled can demand higher resolutions. Areas of lower interest or atmospheric complexity can be modeled with coarser grids. The DoD and DoE have historically taken leads in this area, and civilian modeling efforts can benefit from technology transfer.

Data Needs for Mission Planning and Acquisition Support

Agent-specific data of all types are needed for mission planning and acquisition support. Such data are currently not being captured systematically and are generally not available from a single source for CB modeling.

Modeling Microscale Phenomena and Processes

Modeling of precipitation within weather models continues to be challenging. Models with large grid sizes use parameters to account for convective processes. Some studies have indicated that this approach does not adequately forecast precipitation events.⁹ Models with 10-kilometer grids require explicit cloud and precipitation microphysics. Better understanding of the atmospheric processes that produce phenomena such as precipitation is needed to substantially reduce forecast errors for mesoscale models. Both the initiation and the growth and decay of atmospheric processes that result in precipitation need better understanding and formalization. In some applications, the time step of the model also needs to be adapted for proper resolution of precipitation and other micro atmospheric phenomenon such as fog and dewfall.

Modeling Stable Boundary Layers

Militarily significant releases can be expected to occur during nighttime hours. Nighttime is also generally associated with stable boundary conditions in the atmosphere. Currently, we do not fully understand the transport and dispersion of pollutants in a stable

⁹ Park et al., May 2000; Abbs, May 2000

boundary layer. In addition, knowledge of downslope flows and topographic damming is not well-developed.

Computational Fluid Dynamics and Vector Processing Machines

Our understanding of stable boundary layers should be much better in five years.¹⁰ Computational Fluid Dynamics (CFD) hold promise in being able to characterize boundary layers accurately. The problem with widespread use of CFD for many modeling domains, however, is the problem with computational burden. Modelers in Japan and Europe are moving ahead with CFD models. The Japanese supercomputers use a vector architecture that allows CFD modeling for large, complex applications. The US laws do not apply importation of these computers. (Editor's note: please see Comment section for additional information on this topic.)

Large Eddy Simulations Modeling

Large Eddy Simulation (LES) modeling is important to properly characterize the transport of pollutants under stable conditions. Turbulent Kinetic Energy (TKEs) must be properly represented for its role in transport in these models.

Diagnostic Flow Models

Diagnostic flow models are beginning to be employed at detailed levels. This can provide better accuracy and make modeling at the 100-meter scale tractable.

Transport, and Dispersion, Fate and Terrain

Current Capabilities

The workshop participants assembled the areas of transport, dispersion, fate, and terrain into a single area of interest. There was some discussion on the relative maturity of the transport and dispersion models.

The workshop participants cautioned against. They emphasized that DoD has had a policy of testing its models in situations that are simple and where the models are most likely to work well. It has not frequently tested its models in more realistic “real-world” situations. The civilian agencies have done this, however, and they are aware

¹⁰ Bach, July 2000

that the model predictions are greatly at risk because we do not yet understand how to predict dispersion in complex terrains such as coastal and urban settings (where most people live).

The civilian atmospheric modelers at the workshop emphasized that the DoD may believe that its models work well and that, in limited circumstances, they probably do. To the knowledge of the workshop participants, however, DoD has not tested models in situations like those likely to be encountered in battlefield conditions.

Scientific and Technical Directions

Community Outreach

The civilian modelers emphasized that the DoD community seems to suffer from isolation from the civilian research community. They detected several areas where the DoD scientists appeared to be just discovering things that have long been a part of the civilian arsenal. They did admit that there are also instances where the DoD scientists have developments that are ahead of the civilian sector.

The civilian researchers strongly suggested an immediate linkage of the DoD community with the community model development effort—the Weather Research and Forecasting model (WRF). A linkage at this time would permit some input into the way that WRF is being structured. They emphasized that this step must be taken immediately, as major design decisions are currently being made by the WRF team.

Removal Mechanisms Modeling

One area of concern is the modeling of removal mechanisms. Chemicals interact with the background aerosols, and there is scavenging as a result of precipitation, and there is dry deposition. In addition, microscale processes such as fog, dewfall, and clouds reduce pollutants, leaving less to disperse further. Current modeling efforts do not generally treat these phenomena adequately. There is need for a new body of experimental data pertaining to the areas of interest, and a determination of which studies could satisfy the data requirements of models now under development. Single dispersion experiments in simple circumstances do not help us understand very much about cities, coastal regimes, complex topography, etc. Ensembles of studies are needed.

Dose Response

Current Capabilities

Nearly all workshop participants agreed that dose-response is an area of severe concern. There is currently a lack of generally-accepted dose-response values for many chemical and biological agents, both military and industrial forms. The effects of agents on populations by age, gender, and health status is not well understood. Because human testing is not possible, great uncertainties will continue in the relationship between expected dose and response outcomes. The true dearth of modern, experimentally-derived dose-response datasets is inescapable, although recent reassessment of the nonlinear time-concentration problem is encouraging. Sublethal and even subclinical effects data are not particularly well-suited for translation to the detailed formalism required by quantitative exposure models. (*See Rickmeier et al., 2001 for key R&D published after workshop.* - Ed.)

Scientific and Technical Directions

Testing and Data Extrapolation

The workshop participants noted that limited animal testing is possible to address this problem. Also, extrapolation to humans is supported by other techniques (cellular receptors, adhesion, in-vitro, in-vivo). They urged strong efforts to pursue innovative approaches to data collection.

Low Dose Effects

Effects of low doses on populations remains an intractable problem. In comparison with other battlefield hazards, how can risks from low or intermittent "regulatory" exposures be assessed?

Data Response for Militarily Significant Activities

For military purposes, it is important to define the dose-response relationships for classes of human activities and for varying protective circumstances (e.g., gloves, suits, MOPP gear, etc.). However, these data are also scarce, and animal testing may not be applicable.

Population and Epidemiology

Current Capabilities

If some of the event data are known and the agent is understood, it is possible to identify the populations exposed immediately after the event, within some error bands. However, there are grave difficulties in modeling new diseases and new agents: ignorance may be irreducible.

Even more difficult is the separation of “normal” diseases from deliberate acts of biological terrorism.¹¹ There has been only limited data gathering on the spread of some infectious diseases. The CDC has done a large portion of the scientific work for modeling the spread of the infectious diseases. Recent work by a workshop participant has focused on modified SEIR (susceptible, exposed, infectious, recovered) models for diseases such as Ebola HF, smallpox, and plague. The models using time-varying rates of disease transmission derived by a Monte Carlo treatment of real historical outbreak data (see J. Bombardt, IDA Paper P-3488).

Scientific and Technical Directions

Database of Genotypes

The workshop participants emphasized the need to develop a database of disease organism genotypes by regions and countries. This would aid in the analysis and attribution of pathogens to the area in which similar pathogens exist.

Epidemiological Models

There is a need to continue development and validate time-dependent models of the spread of infectious diseases (e.g., effect of transit systems, population interactions). These models should explicitly incorporate geographic spread as well as the time course of disease.

Medical Surveillance Systems

The ability to detect an ongoing biological attack relies heavily on medical surveillance systems. There is a need to integrate medical surveillance systems more tightly with command and public health elements, and share timely data on evolving disease patterns. The surveillance system also needs validation to ensure that it can provide

¹¹ National Intelligence Council, September 2000

high-quality, verified data quickly and allow modeling of the spread of a disease.

Uniform High-Quality Diagnostics

Uniform high-quality diagnostics is a problem in both reconstruction and medical surveillance; because of this, there are front-end uncertainties. Since initial data on population and epidemiology come from an individual physician diagnosing a patient at a time, considerable uncertainties may exist in the overall population and epidemiological modeling. Physicians are beginning to learn about bio-terrorism and diagnosis of biological attacks through the training provided by the DoD Domestic Preparedness program.

Human Behavior Modeling

Although human behavior modeling is critical for successful modeling on a larger scale, the actions of humans are more complex and less susceptible to mathematical formulations than the processes of the atmosphere. Because human population movements and activities are expected to have a strong influence on the spread of diseases, the workshop participants spent considerable time and attention on the issue of the need and complexity of human behavior modeling.

Even for chemical agents where the effects are expected to be relatively immediate, the forecast of chemical agent plumes may be over-shadowed by the “worried sick” presenting at area hospitals. The Aum Shinrikyo event indicated that almost 14 to 15 times as many people as were estimated to be actually symptomatic will show up at hospitals, requesting treatment.

Economic Impacts Modeling

There are other secondary and tertiary impacts of chemical or biological events. For example, business interruptions, agricultural quarantines, and other economic impacts can be expected over a region greater than the area of direct impacts. These must be taken into account in modeling for decision support.

Agriculture and Biota

Current Capabilities

The workshop participants had considerable ambivalence about whether or not “Agriculture and Biota” is really a DoD mission. One of the participants noted that “the Army travels on its belly,” and that

anything that jeopardizes the food supply could affect military operations. (According to open-press reporting, Russia had weaponized anti-plant and anti-animal agents.) The issue largely resides with civilian agencies responsible for agricultural and environmental issues, such as USDA and EPA. If large-scale destruction of crops or animals were involved, however, the DoD and regulatory agencies could also become involved.

Whether animal or plant diseases are intentional, accidental, or part of natural mutagenic processes, there is considerable concern about food supply assurance. If diseases cross the species barrier and affect humans, there will be severe concerns, both about people's immediate health and safety and about secondary effects such as contamination of blood supplies.

Agriculture and biota are the "canaries in the mine." They are the early indicators of problems that may affect human beings. However, it is hard to learn how an animal disease may spread in the human population. Diseases spreading rapidly in these populations result in policies to destroy potentially-diseased animal and plant stocks. The workshop participants believed that the first insult cannot be stopped. However, through surveillance and modeling, the process can be understood enough to intervene and take actions.

One participant observed, "Foot and Mouth Disease (FMD) is a biological attack in slow motion." Still, it was not clear to workshop participants if the current capability can be scaled up to modeling multiple, multi-point deliberate biological acts.

(Editor's note: the FMD epidemic struck Great Britain and the EU just a few weeks after this workshop. As the disaster grew in scope and damage, modeling became a key tool in fighting the disease. See <http://www.maff.gov.uk/inf/newsrel/2001/010323a.htm> "Foot and Mouth Disease: Epidemiological Forecasts". Model analysis helped to determine the operational policy of destroying animals on infected and non-infected but neighboring farms within 48 hours. Over 1500 troops were mobilized as of 9 April 2001 to assist veterinary authorities in dealing with destruction and disposal of animals. See www.newssearch.bbc.co.uk/hi/english/uk/newsid_1264000/1264341.stm)

Scientific and Technical Directions

Microbial Genomics

DNA has revolutionized human medicine. Microbial genomics holds the promise for providing the same quantum leap in capability for the

complex interactions of host-pathogens.¹² Workshop participants encouraged the continuing federal investment in microbial genomics. There are many benign medical and ecological reasons to study microbes. The potential for microbes to be used in biological warfare makes it important to be able to detect, characterize and attribute (if such is possible) the microbe to specific regions around the world or to specific actors. There is a deterrence quality to an active forensics program; when matched with intelligence, it is a potent weapon to prevent biological attacks.

Biological Forensics

Biological forensics will require a rigorous, consistent approach to modeling in order to satisfy scientific and legal standards. Biological forensics must be defensible. Modeling will need to use trajectory analysis; such trajectory analysis generally needs a sophisticated recording system that can allow modeling of spread in space and time.

Digital Database of Economically Important Agriculture and Biota

Since the concern is also with plant and biota, there needs to be a digital database of economically important agriculture and biota. Such data are available from both public agencies and commercial sources; however, this data needs to be pulled together into an integrated set.

Materiel

Current Capabilities

Protective equipment used by U.S. forces needs to be tested and modeled in force on force simulations. There are some examples of good use of modeling and simulation for various modeling domains. The Long Range Bio Standoff Detector included an excellent simulation capability. The CB Simulator and the Virtual Emergency Response Training System (VERTS) provide commercial, entertainment-industry type simulation environments. The immersive virtual environment of VERTS is especially effective for training. The consensus of the workshop participants was that this discipline is not technologically limited but is both process-inhibited and organizationally inhibited.

¹² National Science and Technology Council, 1996

Scientific and Technical Directions

Testing Methodologies

Testing methodologies are very important for properly capturing the behavior of materiel. Although inadequate in the 1980s when many data sets were gathered, testing methodologies have been refined since; still, they are not totally adequate. Testing is currently focused on “proving the positive” rather than exploring the unexpected behavior of materiel. Also, testing to requirements does not provide the entire range of test data needed for use in simulation models.

Virtual Proving Grounds

Virtual Proving Grounds have not realized their true potential yet. Accurate modeling and simulation can play a pivotal role in such testing through portrayal of CB agent effects. The lessons of simulation-based acquisition are relevant: it is much less expensive to discover a system shortfall in virtual testing rather than after production and deployment. When materiel developers to construct virtual representations of their systems, many real-world insights are gained through the process of functional decomposition and software representation.

Virtual Prototyping of Components

The Joint Service Integration Group (JSIG) is at the front-end of the process of defining materiel requirements. The analysis of alternatives at this front end should be driven by virtual prototyping of components and requirements. This will require investing in creating acquisition-specific models for CB materiel.

Collaboration with Entertainment Industry

The entertainment industry is rapidly enhancing its ability to deliver high-fidelity, immersive environments. Considerable resources are being deployed to develop capabilities. DoD needs to continue to collaborate with the entertainment industry in order to leverage its technical skills for military simulations.

Miscellaneous Observations

The CB Modeling & Simulation Workshop began with participants identifying eleven areas that defined the “end-to-end” modeling sought. By the time of the completion of this white paper, the eleven areas had become compressed into six, as listed below:

- source-term, intelligence integration
- weather, transport, dispersion, fate, and terrain

- dose-response
- population and epidemiology
- agriculture and biota, and
- materiel

A consistent thread of the workshop was that artificial modeling barriers do not adequately represent closely connected process. Also, it was stated repeatedly that chemical and biological agents need to be treated separately in certain key respects such as persistence, contagion, and transformation in the environment. However, weather and dispersion as they affect aerosol transport and fate are common to both types of agents.

Requirements from each DoD modeling domain need to be considered for modeling and simulation. A transport and dispersion model for exercises and training may not need as much “true” fidelity in terms of representing a precise meteorological forecast as would the same model used during military operations. A forensics application may need to use the highest fidelity, as there is both time and interest in modeling a specific event or series of events as accurately as possible.

If users are to accept the modeling and simulation products, they must then have adequate training. "Deployed" personnel need to use or access outputs from CB models; this requires a comprehensive and sustained program of initial and refresher training.

Users need to inform modeling and simulation development. With that said, workshop participants strongly emphasized that users should not define the detailed criteria of models. Instead, they should provide flexible and over-arching requirements. The concern, workshop members believed, was that users may define very detailed requirements based on current scientific capabilities. Leap-frogging scientific breakthroughs can be stifled by such prescriptive criteria.

Modeling is needed to improve other models. Parametric models need to be developed to test the accuracy and sensitivity of other models. These parametric models can show where model improvements may be needed.

The civilian workshop participants noted that there are significant differences between civilian and DoD modeling approaches. In some areas, the civilian modelers have moved substantially ahead. These areas include the integration of atmospheric forecast models with transport-and-dispersion models, as well as ensemble and

probabilistic modeling. There is considerable benefit in the DoD and the civilian modelers working together.

Modeling Domains and Scientific Challenges

On the final day of the workshop, panel members identified variations in the level of scientific challenge posed by the modeling disciplines. Gradings of red, yellow, and green were used, as shown in Table 1:

Table 1: Gradings Showing the Level of Scientific Challenge Posed by Modeling Disciplines

Color	Meaning
Red	Critical technical leaps needed
Yellow	Significant technical improvements needed
Green	Technically okay for the modeling domain. New requirements may change this to “red” or “yellow.”

Workshop participants identified the current situation for each of the modeling disciplines for the various application domains. Then, the expected improvements by 2010 were identified, as shown in the following Figure 3. This future status presupposes appropriate financing for improvements to occur. The colors are merely an indication of the technical challenges, not fiscal or otherwise.

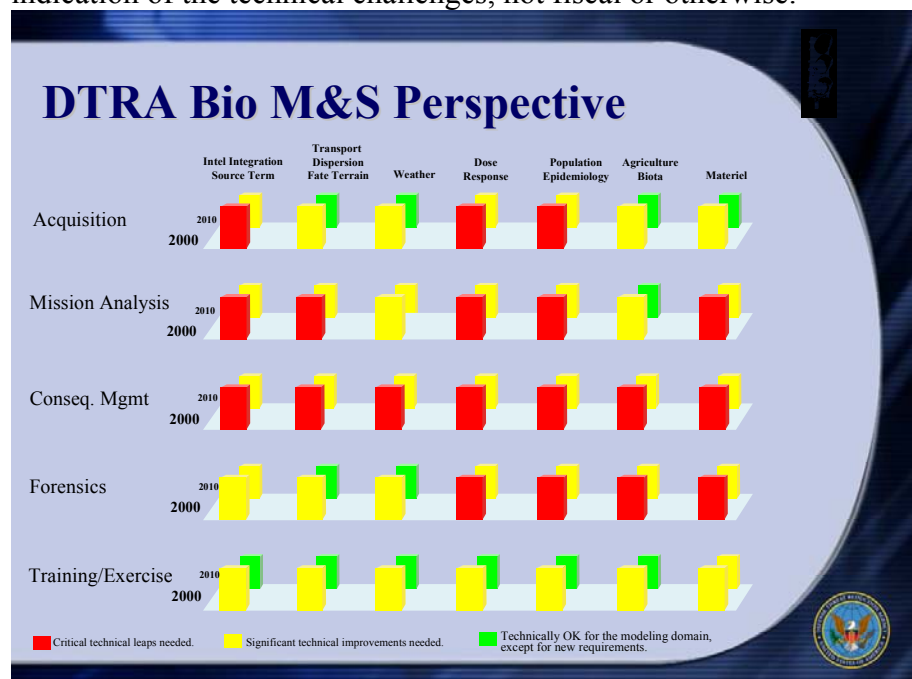


Figure 2: Expected Improvements by 2010 that were Identified at the Workshop

Comments from Participants

Dr. Jay Davis posed this question to the National Science Foundation:

Is there any technical basis for the following assertion? "The lack of large vector machines has put us behind the Europeans and Japanese in CFD modeling".

Dr. Charles Koelbel, Advanced Computational Research Program Director, replied as a consultant to the workshop:

To oversimplify the situation: There are many parallel CFD codes that perform to their creators' and users' satisfaction. Explicit methods work well in parallel, and are appropriate for many situations. However, they may require very small timesteps for stability, making them a poor choice for (e.g.) long-range weather forecasts. Implicit methods can be made to work in parallel, but not without pain. How much pain is application-dependent. Implicit methods are generally seen as the more modern CFD algorithms.

Running efficiently in parallel usually requires rethinking the algorithms. This leads to many comments that parallelism will never work for application X. (The same was said of vector machines, of course. But that was 25 years ago and the people who said it have mostly retired. Also, vector machines *could* be used as scalar processors with "only" a 10x slowdown; that's not true of scalable parallel machines.) Whether the comments reflect an unwillingness to rethink or a serious, unsuccessful attempt to rethink varies.

Some of those doomsday comments may in fact be true. There are theoretical bounds on parallelism, which have about the same relation to ASCI-class machines as bounds on Turing Machines do to your PC's performance. (Typical Turing bounds include NP-complete problems, so they're not *completely* irrelevant...) Few of the "parallelism won't work" comments are backed by such proofs, though. It is certainly true that today's parallel machines achieve a lower efficiency (% of peak) in practice than vectors. Whether that is inherently true, or a function of 10-20 years more experience in vectorization than parallelization, is hard to say.

From Dr. Bruce Hicks

ATMOSPHERIC PROCESSES, TRANSPORT AND DISPERSION

The DoD/DTRA community seems to suffer from isolation from the civilian research community. I detect several areas where the DoD scientists appear to be rediscovering things that are already a part of the civilian arsenal, but there are also instances where the DoD scientists have developments that are ahead of the civilian sector.

As a simple first step towards generating the capacity to gain access to the civilian sector, I strongly suggest an immediate linking with the community model development effort -- the Weather Research and Forecasting model (WRF). A linkage at this time would permit some input into the way that WRF is being structured. It is critical that this step be taken immediately, since major design decisions are being made by the WRF team at this time.

Further, I recommend that the distinction between "weather" and "transport and dispersion" be slowly eliminated from the thinking. This distinction is a carry-over from the days when weather models provided wind field data that were then used to drive dispersion routines. In practice, this separation caused difficulties because many of the basic data needed by the dispersion routines were not archived by the weather forecasting community. The next generation of mesoscale model will solve all such problems, by combining the transport and dispersion capabilities with the forecast codes. (Many models do this already.) In this way, the concept of an ensemble probabilistic forecast will extend all the way to the dispersion products.

Each of the following is a red light area, currently requiring attention. In some of these we currently know enough only to be sure that we are making huge errors.

Meteorology

Use of standard forecasts to address local situations

Grid cell compression

Exploitation of adaptive grid techniques (DoD has historical led)

Ensemble approaches (DoD seems to prefer single-model approaches; I would use the Navy model for the oceans, and use civilian models for the land.)

Probabilistic approaches (It is said that battlefield commanders do not know how to weigh probabilities. I do not believe this.) Take precipitation into account, also fog and dewfall

Flows in complex terrain

Urban areas (Need a new generation of models. Adaptive grids possibly best for stable conditions, at least. I do not favor adaptive grids for unstable conditions.)

Hills
Coastal
Islands
Identification of safe and dangerous areas

Stable flows

Downslope flows
Damming
Nighttime situations
Identification of safe and dangerous areas

Removal mechanisms

Interactions with background aerosol
Precipitation scavenging
Roles of fog, dewfall, and clouds
Dry deposition

Inside and outside buildings

Dispersion rates within buildings
Exchange with outside atmosphere
Identification of safe and dangerous areas

Source location

Back trajectories
Receptor modeling
Hybrid methodologies

In addition to the above "red light" topics, there are over-riding needs: community modeling efforts and field data collection.

Community modeling

There would be great profit if the DoD effort were to be coupled with Parallel efforts in other agencies. A simple way to achieve this would be to become a partner in the community modeling efforts already under way; e.g. WRF and Models-3.

Observations

There is need for a new body of experimental data pertaining to the areas of interest, and which satisfies the requirements of models now under development. Single dispersion experiments in simple circumstances do not help us understand very much about cities, coastal regimes, complex topography, etc. Ensembles of studies are needed.

I compared notes with others who attended the meeting, after I prepared my summation above. I found some agreement, but not universal. It was mentioned, however, that the meeting concluded

with allotting green and yellow to most of the dispersion aspects of the problem. I need to disagree with this, for the reason that I emphasized during the meeting.

DoD has had a policy of testing its models in situations that are those addressed by the current models. It has not tested its models in situations like the real world in the Balkans, for example. However, the civilian agencies have invested heavily in complex terrain dispersion studies and are well aware that the model predictions are greatly at risk.

DoD certainly thinks that its models work well, and in limited circumstances they certainly do, but DoD has not tested them in situations like those likely to be encountered in many battlefield conditions. (To my knowledge, anyway.) A blanket endorsement of current DoD models will be looked at quite askance by those on my side of the fence. We need to make sure that DoD is not glaringly out of step with the rest of the world. My point about bringing weather forecasting and dispersion together in the same code is not shared by all. In fact, I suspect that this might be another point of departure for the DoD and civilian communities. Certainly, the use of a combined modeling approach is being tested in many places. Whatever approach DoD should elect to take should probably be such that it does not make DoD look greatly at odds with the scientific community at large.

From Dr. Arthur Hopkins

Validation and verification processes: I think OSD can and should certify for use, but we (the community) need to devise and execute auditable, peer-reviewed V&V processes to help underwrite OSD efforts. They'll help establish credibility and guide R&D investment planning for modernization. Configuration management should also be considered.

From Dr. Steven Hanna:

The color-coded grading does not represent a consensus, even though the current text implies that there was much discussion about each grade assignment. We spent only about an hour on the entire grading discussion, and only a small fraction of the group gave their opinions and no vote was taken.

I think it was Bruce Hicks who suggested words related to how civilian models and field experiments were ahead of DoD activities in these areas. I don't think this is true anymore. I feel that the DTRA-sponsored SCIPUFF model is the best puff dispersion model from a scientific viewpoint and it has been improved so that it is applicable to a very wide variety of release scenarios and geographic domains. Furthermore, it has been evaluated against more tracer datasets over a wider range of scales and scenarios than any EPA or NOAA model. DoD experiments such as Dipole Pride 26 represent real-world complex terrain situations typical of what might be found in a real battlefield situation.

The uncertainties in complex modeling systems can be assessed using Monte Carlo uncertainty analysis. The methodology would be applicable to most modeling scenarios, including those discussed at the DTRA workshop. Over the past few years, I have participated in several peer reviews of DOE and CDC dose reconstruction efforts at DOE National Labs, and they seem to always use a Monte Carlo uncertainty approach, applied to the end-to-end modeling system (i.e., from emissions models, through transport and dispersion models, through dose models, and finally through health effects models) (Uncertainties in predicted ozone concentrations due to input uncertainties for the UAM-V photochemical grid model applied to the July 1995 OTAG domain, Hanna, S.R., Zhigang Lu et al., 2001, Atmospheric Environment, vol. 35, 891-903).

I also mentioned at the workshop that the EPA has a rapidly increasing interest in Monte Carlo uncertainty methods, and has prepared a Guidelines Report (Chang, S., 1997, www.epa.gov).

From Dr. Jon Mercurio:

(Please note) a recent report "A Study of Turbulence and Dispersion in the Atmospheric Boundary Layer Above Heterogeneous Land Surfaces" by Roni Avissar. This report documented work supported by the US Army Research Office and provides a partial basis for the comments regarding modeling scales. In particular, it illustrates, using RAMS in LES mode, the problems of using mesoscale models to characterize the high resolution flows necessary for small scale dispersion simulations.

From the Army perspective, we need rapid response to a battlefield attack. Met models are notoriously slow and produce large data trails. If we wait until an attack occurs to develop the sufficiently high-resolution Meteorological data simultaneous with the T&D

calculations, we are looking at post event processing, more the forensic analysis role than the Tactical decision scenario. It will still be some time before battlefield computers are sufficiently large and fast to accommodate such ideal conditions. In the real battlefield, it seems that it will be sometime before we can hope for real time integrated Met and T&D calculations.

From Dr. Jerry M. Davis:

I think this is an excellent job in capturing the consensus views expressed by the participants at the workshop. While I read the entire report, I gave special attention to the sections on atmospheric sciences. At this point, I think those sections are fine. I do think that some term other than "weather" should be used in most instances in the report (e.g., "meteorological models" instead of "weather models"). In addition, while Bayesian methods were mentioned in passing, I believe that Bayesian decision analysis could be quite useful in a number of instances. But this is not a critical addition to the report at this point.

From Dr. Jay Boris:

The importance of source term is overstated. Natural uncertainty coupled with strong insensitivity because of sharp cloud edges means limited accuracy is needed here. It is important to do physics before statistics. Physics of fluid dynamics is highly nonlinear so applying statistics too early is very dangerous. There was too much attention to atmospheric dynamics relative to other areas of higher priority. Due to the poor state of realistic urban modeling, "Transport, Dispersion, Fate and Terrain" should be rated as "High" priority. The current push to validate and accredit DoD models makes it very difficult to get an honest assessment of their shortcomings from those most knowledgeable. As a result, problem areas are downplayed dangerously.

From Dr. Jeffrey Grotte:

While modeling might play a role (in the immediate aftermath of a release), I think the response would be based almost entirely on real world events. Thus, responding to a chemical attack would be based in detector indicators and effects. The role of models is probably overstated. What might be important here is that unless models reach a certain threshold of fidelity, they will probably be peripheral.

Perhaps an important point of this workshop is that unless the data and models can reach that threshold, their utility will continue to be very limited.

One area that has to be addressed is training and education for commanders and warfighters. Unless they understand the models and what the outputs mean, including their strengths and limitations, model results will always be “black magic,” used to produce pretty pictures but not used to guide decision making.

If we know that some type of missile has been used, and we have developed appropriate parameters for that weapon (not that easy to do) then we can have a reasonable source term. If it is totally covert attack, revealed only by its effects, it will be very difficult.

Monte Carlo analysis: Often we know just as little about the (parameter) distribution as we do about the variable values. Moreover, specifying the distribution does require specifying particular values, such as mean and standard deviation. While Monte Carlo is useful, it is not a panacea for lack of knowledge.

(Editor's note: one may specify a uniform distribution with a "min-max" range for any parameter. If such hypotheses are lacking, the parameter should be omitted from any model, and perhaps is best served by a discovery process, rather than use as a blind fitting element in a model.)

For fixed site or urban applications, microscale models are vitally important. Our failure to really apply them results from their complexity. Important phenomena include evaporation, absorption of agent into materials, chemical reactions with typical military surfaces, such as paints. These are critically important for estimating hazards in the field and should be included here. The effects of temperature on agent behavior appear to be poorly understood as well. In addition, the phenomenology of agent pickup and transfer is also critical to understand. The percentages of agent that are picked up off of various surfaces (such as grass) onto equipment (such as boots) and are deposited on other surfaces (such as vehicle floor mats) are important to the determination of hazard conditions.

Current models provide little capability to provide spatial information on disease spread. This type of modeling, especially if it can take into account population movements (not just transit systems), would seem at first glance to greatly enhance our ability to address disease spread. Probably two levels are needed—one at the individual city level and

one at the national level since biological attacks at airports, for instance, could have country-wide implications.

The use of antibiotics in animal feed has been a very visible area of concern. I expect there are a number of vaccines used for commercial animals as well. Plants are also bred for disease resistance, which can be considered a form of prophylaxis.

DoD talks the talk about verification and validation, but does not walk the walk. Current approaches are unworkable. We need a whole new approach to validation, which will probably include testing in real-world areas, not just at Dugway Proving Grounds.

From the DTRA Computing Team:

The Scientific Computing (TDANP) team provides high performance computing resources for agency research efforts. These resources are provided at no cost to Agency programs. We provide the computing platforms, software, technical support and communications where needed and within reason. We also provide classified computing which requires a long lead time to establish the classified connections. The majority of our users are contractors that the Agency employs however, technical monitors can have access as well. Scientific Computing provides for the Agency access to the following computing:

DTRA - Telegraph Road

Cray SV1A Computer: q.dtra.mil (Unclassified)

Unicos 10.0.7 Operating System

16 CPU's @ 1.2 Gflops peak performance per CPU

16 Gbytes memory

Storagetek WolfCreek 9360 Robotic Tape Silo

High Performance Computing Modernization Program (HPCMP)

<http://www.hpcmo.hpc.mil/>

The DoD HPC Modernization Program provides advanced hardware, computing tools and training to DoD researchers utilizing the latest technology to aid their mission. The website has a complete listing of hardware, software, training and other research opportunities.

Los Alamos National Laboratory (LANL)

SGI Origin 2000 theta.lanl.gov (Unclassified)

IRIX 6.5 Operating System

2 Processor Origin 200 Front End

96 Processor Origin 2000 @ .5 Gflops peak per CPU

114 Gbytes memory

Advanced Computing Lab (ACL) Unclassified ASCI system

SGI Origin 2000 nirvana.lanl.gov

IRIX 6.5 Operating System

2 Processor Origin 200 Front End

2048 Processor Origin 2000 @ .5 Gflops peak per CPU

576 Gbytes memory

Storage: High Performance Storage System (HPSS), Common File System (CFS)

References

Abbs, Debbie, May 2000. The effect of convective parameterization and model resolution on quantitative precipitation forecasts of extreme rainfall events, in *Proceedings of the 4th RAMS Users Workshop*. Mission Research Corporation.

Avissar, Roni. "A Study of Turbulence and Dispersion in the Atmospheric Boundary Layer Above Heterogeneous Land Surfaces", U.S. Army Research Laboratory.

Bach, W.D., July 2000. "CASES-99 field experiment in stable boundary layers" in Fourth GMU Transport and Dispersion Modeling Workshop. George Mason University.

Bombardt, John. Contagious Disease Dynamics for Biological Warfare and Bioterrorism Casualty Assessments. Institute for Defense Analyses, IDA Paper P-3488, Feb. 2000.

Camelli, F., and R. Lohner, 2000. Flow and dispersion around buildings: an application with FEFLO. *Proceedings for ECCOMAS 2000*. European Congress on Computational Methods.

Chang, S., 1997. Guiding principles for Monte Carlo analysis. EPA/630/R-97/001, ORD, Risk Assessment Forum, USEPA, Washington, DC 20460.

Cybyk, B. Z., J. Boris, T. Young, C. Lind, A. Landsberg. A detailed contaminant transport model for facility hazard assessment in urban areas. AIAA 30th Plasmadynamics and Lasers Conference.

Cybyk, B. Z., J. Boris, T. Young. Coupling of External Winds and Recirculations with Interior Contaminant Release Modeling. American Meteorological Society.

Davis, J. M., C. E. Main, and R. I. Bruck. 1981. Analysis of weather and the 1980 blue mold epidemic in the United States and Canada. *Plant Disease* 65:508-512.

Davis, J. M. and C. E. Main. 1984. A regional analysis of the meteorological aspects of the spread and development of blue mold on tobacco. *Boundary Layer Meteorology* 28:271-304.

Davis, J. M., C. E. Main, and W. C. Nesmith. 1985. The biometeorology of blue mold of tobacco. Part II, The evidence for long-range sporangiospore transport. IN D.R. MacKenzie, C.S. Barfield, G.G. Kennedy, and R.D. Berger (eds.), *The Movement and Dispersal of Agriculturally Important Biotic Agents*. Baton Rouge, Louisiana: Claitor's Publishing Division.

Davis, J. M., and C. E. Main. 1986. Applying atmospheric trajectory analysis to problems in epidemiology. *Plant Disease* 70: 490-497.

Davis, J. M. 1987. Modeling the long-range transport of plant pathogens in the atmosphere. *Annual Review of Phytopathology* 25:169-188.

Davis, J.M., C.E. Main, and W.E. Nesmith. 1990. The aerobiological aspects of the occurrence of blue mold in Kentucky in 1985. IN (C.E. Main and H.W. Spurr, editors) *Blue Mold Disease of Tobacco. Proceedings of a Symposium held at Raleigh, NC, February 14-17, 1988*. pp 55-71.

Davis, J.M. and J.F. Monahan. 1991. A climatology of air parcel trajectories related to the atmospheric transport of *Peronospora tabacina*. *Plant Dis.* 75:706-711.

Environmental Protection Agency, March 1997. Guiding principles for Monte Carlo analysis. Washington, DC.

Hanna, S.R., 1999. Parameterizing urban climate in dispersion models. Keynote Address published in *Proceedings of International Congress on Biometeorology and International Conference on Urban Climatology*, Sydney, AU, 11-15 November, 1999.

Hanna, S.R., and R.E. Britter, 2000. Effects of urban and industrial roughness obstacles on maximum pollutant concentrations. *Proceedings, Millenium NATO/CCMS International. Technical Meeting on Air Pollution Meteorology and Its Applications*. Boulder, CO, 14–19 May 2000.

Hanna, S.R., R. Yang, and X. Yin, 1999. Evaluations of Numerical Weather Prediction (NWP) models from the point of view of inputs required by atmospheric dispersion models.” *J. Environ. Poll.*

Hanna, S.R., Zhigang Lu, H. Christopher Frey, Neil Wheeler, Jeffrey Vukovich, Saravanan Arunachalam, Mark Fernau and D. Alan Hansen, June 2000. Uncertainties in predicted ozone concentrations due to input uncertainties for the UAM-V photochemical grid model. Applied to the July 1995 OTAG Domain, to be published in *Atmospheric Environment*.

Haydon, D.T., M. E. J. Woolhouse, R. P. Kitching. An Analysis of foot-and-mouth disease epidemics in the UK, *IMA Journal of Mathematics Applied in Medicine & Biology*, Vol. 14, 1997.

Main, C. E., J. M. Davis, and M. A. Moss. 1985. The biometeorology of blue mold of tobacco. Part I: A case study in the epidemiology of the disease. IN D.R. Mackenzie, C.S. Barfield, G.G. Kennedy, and R.D. Berger (eds.), *The Movement and Dispersal of Agriculturally Important Biotic Agents*. Baton Rouge, Louisiana: Claitor's Publishing Division.

Merkle, P. B., B. J. Brownawell. 1993. Atmospheric deposition of semivolatile organic compounds to near-shore aquatic environments: simulation of air-water exchange dynamics and cycling. 25th Annual Mid-Atlantic Industrial and Hazardous Wastes Conference, University of Maryland, College Park, MD.

Mollison, Denis (Ed.) *Epidemic Models: Their Structure and Relation to Data*. Cambridge University Press, Publications of the Newton Institute, 1995)

National Center for Atmospheric Research, Mesoscale and Microscale Meteorology Division, October 2000. Science plan: five years and beyond.

National Intelligence Council, September 2000. Modeling the spread of infectious diseases—summary of an open conference of US researchers. Scientific & Technical Intelligence Committee.

National Science and Technology Council, 1996. Interagency report on the federal investment in microbial genomics. Biotechnology Research Working Group.

NUREG 1150: "Severe accident risks: an assessment for five U.S. nuclear power plants," U.S. Nuclear Regulatory Commission, 1990, NUREG-1150.

Office of the Federal Coordinator for Meteorological Services and Support, 2000. Proceedings of the workshop on multiscale atmospheric dispersion modeling within the federal community, June 6-8, 2000.

Park, Y.Y., T.-Y. Lee, J.-W. Kim, S.-Y. Park, Y.-J. Noh, S.-H. Park, and D.-I. Hwang, May 2000. Sensitivity of heavy-rain simulation to the treatment of model physics, in *Proceedings of the 4th RAMS Users Workshop*. Mission Research Corporation.

Rasmussen, Norman C. et al., 1975. Reactor safety study: an assessment of accident risks in the U.S. commercial nuclear power plants, Nuclear Regulatory Commission, NUREG-75/014 (WASH-1400), Washington, DC.

Rickmeier, G.L., McClellan, G.E., Anno, G.A. 2001. Biological Warfare Human Response Modeling. Military Operations Research, V6, No. 3.

Smith, R.L. and Davis, J.M. 1997. Assessing the human health risk of atmospheric pollutants. Proceedings Volume for the 1997 Joint Statistical Meetings, Anaheim (CA), August 10-14, 1997.

Smith, R.S., Davis, J.M., Speckman, P. 1998. Airborne particles and mortality. Pages 91-120 IN Case Studies in Environmental Statistics (editors: Nychka, Piegorsch and Cox). Springer Lecture Notes in Statistics (Volume 132). New York: Springer Verlag. 196 pages.

Smith, R.L., Davis, J.M., and Speckman, P. 1999. Human health effects of environmental pollution in the atmosphere. Pages 91-115 IN Statistics for the Environment 4: Statistical Aspects of Health and the Environment (editors: V. Barnett, A. Stein, and F. Turkman). Chichester: John Wiley and Sons.

Smith, R.L., Davis, J.M., Sacks, J., Speckman, P. and Styer, P. 2000. Regression models for air pollution and daily mortality: analysis of data from Birmingham, Alabama. *Environmetric* 11:719-743.

Styer, P., McMillan, N., Gao, F., Davis, J.M., Sacks, J. 1995. Effect of outdoor airborne particulate matter on daily death counts. *Environmental Health Perspectives* 103: 490-497.

Tehrani, S., R. Lohner and S. Hanna, 2000. Numerical simulation of airflow in the vicinity of several rectangular-shaped buildings and airflow and dispersion around an L-shaped building. *Proceedings, ENVIROSOFT 2000, Eighth International Conference on Development and Applications of Computer Technologies to Environmental Studies*, Bilbao, Spain, 28–30 June 2000.

Yao, C., Arya, S., Davis, J.M., Main, C.E. 1997. A numerical model of the transport and diffusion of *Peronospora tabacina* spores in the evolving convective boundary layer. *Atmospheric Environment* 31: 1709-1714.